WHAT IS CLAIMED IS:

1. A system for calculating a potential of mean force (PMF) score of a protein-ligand complex, the system comprising:

a repulsion-term module that:

accesses one or more parameters useable to calculate a repulsion term useable to calculate a PMF of a protein-ligand atom pair in the protein-ligand complex, the one or more parameters corresponding to an atom-pair type of the protein-ligand atom pair;

using the one or more accessed parameters, calculates the repulsion term useable to calculate the PMF of the protein-ligand atom pair; and

communicates the calculated repulsion term for calculation of the PMF score of the protein-ligand complex.

2. The system of Claim 1, wherein one of the parameters corresponding to the atom-pair type of the protein-ligand atom pair comprises an empirically derived minimum binding-energy distance value corresponding to the atom-pair type of the protein-ligand atom pair.

3. The system of Claim 1, wherein one of the parameters corresponding to the atom-pair type of the protein-ligand atom pair comprises an empirically derived well-depth value corresponding to the atom-pair type of the protein-ligand atom pair.

4. The system of Claim 1, wherein:

a first one of the parameters corresponding to the atom-pair type of the protein-ligand atom pair comprises an empirically derived minimum binding-energy distance value corresponding to the atom-pair type of the protein-ligand atom pair; and

a second one of the parameters corresponding to the atom-pair type of the protein-ligand atom pair comprises an empirically derived well-depth value corresponding to the atom-pair type of the protein-ligand atom pair.

5. The system of Claim 4, wherein a set of a plurality of empirically derived minimum binding-energy distance and well-depth values corresponding to a plurality of protein-ligand atom pairs comprises the empirically derived minimum binding-energy distance and well-depth values corresponding to the atom-pair type of the protein-ligand atom pair, the set of empirically derived minimum binding-energy distance and well-depth values yielding a best agreement with a plurality of actual analyzed protein-ligand atom pairs.

6. The system of Claim 5, wherein the plurality of actual analyzed protein-ligand atom pairs are described in a protein data bank (PDB).

7. The system of Claim 5, wherein the best agreement between the set of empirically derived minimum binding-energy distance and well-depth values and the plurality of analyzed protein-ligand atom pairs is determined according to a plurality of root mean square (RMS) deviations between:

protein-ligand complex structures predicted according to the set of empirically derived minimum binding-energy distance and well-depth values; and

actual analyzed protein-ligand complex structures corresponding to the predicted protein-ligand complex structures;

8. The system of Claim 7, wherein a plurality of sets of empirically derived minimum binding-energy distance and well-depth values are generated and compared with each other to determine the set of empirically derived minimum binding-energy distance and well-depth values yielding the best agreement with the plurality of actual analyzed protein-ligand atom pairs.

9. The system of Claim 7, wherein one or more of the plurality of sets of empirically derived minimum binding-energy distance and well-depth values are generated according to one or more of:

one or more manual processes; and

one or more automatic processes.

10. The system of Claim 9, wherein one of the automatic processes comprises execution of a genetic algorithm.

11. A method for calculating a potential of mean force (PMF) score of a protein-ligand complex, the method comprising:

accessing one or more parameters useable to calculate a repulsion term useable to calculate a PMF of a protein-ligand atom pair in the protein-ligand complex, the one or more parameters corresponding to an atom-pair type of the protein-ligand atom pair;

using the one or more accessed parameters, calculating the repulsion term useable to calculate the PMF of the protein-ligand atom pair; and

communicating the calculated repulsion term for calculation of the PMF score of the protein-ligand complex.

12. The method of Claim 11, wherein one of the parameters corresponding to the atom-pair type of the protein-ligand atom pair comprises an empirically derived minimum binding-energy distance value corresponding to the atom-pair type of the protein-ligand atom pair.

13. The method of Claim 11, wherein one of the parameters corresponding to the atom-pair type of the protein-ligand atom pair comprises an empirically derived well-depth value corresponding to the atom-pair type of the protein-ligand atom pair.

14. The method of Claim 11, wherein:

a first one of the parameters corresponding to the atom-pair type of the protein-ligand atom pair comprises an empirically derived minimum binding-energy distance value corresponding to the atom-pair type of the protein-ligand atom pair; and

a second one of the parameters corresponding to the atom-pair type of the protein-ligand atom pair comprises an empirically derived well-depth value corresponding to the atom-pair type of the protein-ligand atom pair.

15. The method of Claim 14, wherein a set of a plurality of empirically derived minimum binding-energy distance and well-depth values corresponding to a plurality of protein-ligand atom pairs comprises the empirically derived minimum binding-energy distance and well-depth values corresponding to the atom-pair type of the protein-ligand atom pair, the set of empirically derived minimum binding-energy distance and well-depth values yielding a best agreement with a plurality of actual analyzed protein-ligand atom pairs.

16. The method of Claim 15, wherein the plurality of actual analyzed protein-ligand atom pairs are described in a protein data bank (PDB).

17. The method of Claim 15, wherein the best agreement between the set of empirically derived minimum binding-energy distance and well-depth values and the plurality of analyzed protein-ligand atom pairs is determined according to a plurality of root mean square (RMS) deviations between:

protein-ligand complex structures predicted according to the set of empirically derived minimum binding-energy distance and well-depth values; and

actual analyzed protein-ligand complex structures corresponding to the predicted protein-ligand complex structures.

18. The method of Claim 17, wherein a plurality of sets of empirically derived minimum binding-energy distance and well-depth values are generated and compared with each other to determine the set of empirically derived minimum binding-energy distance and well-depth values yielding the best agreement with the plurality of actual analyzed protein-ligand atom pairs.

19. The method of Claim 17, wherein one or more of the plurality of sets of empirically derived minimum binding-energy distance and well-depth values are generated according to one or more of:

one or more manual processes; and

one or more automatic processes.

20. The method of Claim 19, wherein one of the automatic processes comprises execution of a genetic algorithm.

21. Software for calculating a potential of mean force (PMF) score of a protein-ligand complex, the software embodied in computer-readable media and when executed operable to:

access one or more parameters useable to calculate a repulsion term useable to calculate a PMF of a protein-ligand atom pair in the protein-ligand complex, the one or more parameters corresponding to an atom-pair type of the protein-ligand atom pair;

using the one or more accessed parameters, calculate the repulsion term useable to calculate the PMF of the protein-ligand atom pair; and

communicate the calculated repulsion term for calculation of the PMF score of the protein-ligand complex.

22. The software of Claim 21, wherein one of the parameters corresponding to the atom-pair type of the protein-ligand atom pair comprises an empirically derived minimum binding-energy distance value corresponding to the atom-pair type of the protein-ligand atom pair.

23. The software of Claim 21, wherein one of the parameters corresponding to the atom-pair type of the protein-ligand atom pair comprises an empirically derived well-depth value corresponding to the atom-pair type of the protein-ligand atom pair.

24. The software of Claim 21, wherein:

a first one of the parameters corresponding to the atom-pair type of the protein-ligand atom pair comprises an empirically derived minimum binding-energy distance value corresponding to the atom-pair type of the protein-ligand atom pair; and

a second one of the parameters corresponding to the atom-pair type of the protein-ligand atom pair comprises an empirically derived well-depth value corresponding to the atom-pair type of the protein-ligand atom pair.

25. The software of Claim 24, wherein a set of a plurality of empirically derived minimum binding-energy distance and well-depth values corresponding to a plurality of protein-ligand atom pairs comprises the empirically derived minimum binding-energy distance and well-depth values corresponding to the atom-pair type of the protein-ligand atom pair, the set of empirically derived minimum binding-energy distance and well-depth values yielding a best agreement with a plurality of actual analyzed protein-ligand atom pairs.

26. The software of Claim 25, wherein the plurality of actual analyzed protein-ligand atom pairs are described in a protein data bank (PDB).

27. The software of Claim 25, wherein the best agreement between the set of empirically derived minimum binding-energy distance and well-depth values and the plurality of analyzed protein-ligand atom pairs is determined according to a plurality of root mean square (RMS) deviations between:

protein-ligand complex structures predicted according to the set of empirically derived minimum binding-energy distance and well-depth values; and

actual analyzed protein-ligand complex structures corresponding to the predicted protein-ligand complex structures.

28. The software of Claim 27, wherein a plurality of sets of empirically derived minimum binding-energy distance and well-depth values are generated and compared with each other to determine the set of empirically derived minimum binding-energy distance and well-depth values yielding the best agreement with the plurality of actual analyzed protein-ligand atom pairs.

29. The software of Claim 27, wherein one or more of the plurality of sets of empirically derived minimum binding-energy distance and well-depth values are generated according to one or more of:

one or more manual processes; and

one or more automatic processes.

30. The software of Claim 29, wherein one of the automatic processes comprises execution of a genetic algorithm.

31. A system for calculating a potential of mean force (PMF) score of a protein-ligand complex, the system comprising:

means for accessing one or more parameters useable to calculate a repulsion term useable to calculate a PMF of a protein-ligand atom pair in the protein-ligand complex, the one or more parameters corresponding to an atom-pair type of the protein-ligand atom pair;

means for, using the one or more accessed parameters, calculating the repulsion term useable to calculate the PMF of the protein-ligand atom pair; and

means for communicating the calculated repulsion term for calculation of the PMF score of the protein-ligand complex.